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KANTBP 3.1: A program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel and adiabatic approaches ☆,☆☆,☆☆☆

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ABSTRACT

A FORTRAN program for calculating energy values, reflection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach is presented. In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on a finite interval with the homogeneous boundary conditions of the third type at left- and right-boundary points for the discrete spectrum and scattering problems. The resulting system of such equations, containing potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method. The scattering problem is solved with non-diagonal potential matrix elements in the left and/or right asymptotic regions and different left and right threshold values. Benchmark calculations for the fusion cross sections of ^{36}S+^{48}Ca, ^{64}Ni+^{100}Mo reactions are presented. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions of the exact solvable wave-guide model, and also the fusion cross sections and mean angular momenta of the ^{16}O+^{144}Sm reaction.

Program summary

Program Title: KANTBP
CPC Library link to program files: https://doi.org/10.17632/4vm9fhyvh3.1
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Programming language: FORTRAN
Nature of problem: In the adiabatic approach [1], a multidimensional Schrödinger equation for quantum reflection [2], the photoionization and recombination of a hydrogen atom in a homogeneous magnetic field [3–6], the three-dimensional tunneling of a diatomic molecule incident upon a potential barrier [7], wave-guide models [8], the fusion model of the collision of heavy ions [9–11], and low-energy fusion reactions of light- and medium mass nuclei [12] is reduced by separating the longitudinal coordinate, labeled as z, from transversal variables to a system of second-order ordinary differential equations containing the potential matrix elements and first-derivative coupling terms. The purpose of this paper is to present a program based on the use of high-order accuracy approximations of the finite element method (FEM) for calculating energy levels, reflection and transmission matrices and wave functions for such systems of coupled-channel second order differential equations (CCSODEs) on finite intervals of the variable $z \in [z_{\min}, z_{\max}]$ with homogeneous boundary conditions of the third-type at the left- and right-boundary points, which follow from the discrete spectrum and scattering problems.

☆ The review of this paper was arranged by Prof. N.S. Scott.
☆☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).
☆☆☆ We dedicate this article to the 75th anniversary of the birth of professor M.S. Kashchiev. He was one of the creators of the first versions of the KANTBP program.

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Solution method: The boundary-value problems for the system of CCSODEs are solved by the FEM using high-order accuracy approximations [13,14]. The generalized algebraic eigenvalue problem $\mathbf{AF} = E\mathbf{BF}$ with respect to pair unknowns $(E, \mathbf{F})$, arising after the replacement of the differential eigenvalue problem by the finite-element approximation, is solved by the subspace iteration method [14]. The generalized algebraic eigenvalue problem of a special form $(\mathbf{A} - E\mathbf{B})\mathbf{F} = \mathbf{DF}$ with respect to pair unknowns $(\mathbf{D}, \mathbf{F})$ arising after the corresponding replacement of the scattering boundary problem in open channels at fixed energy value, E, is solved by the $\mathbf{LDL^T}$ factorization of the symmetric matrix and back-substitution methods [14].

Additional comments including restrictions and unusual features: The user must supply subroutine POTCAL for evaluating potential matrix elements. The user should also supply subroutines ASYMEV (when solving the eigenvalue problem) or ASYMSL and ASYMSR (when solving the scattering problem) which evaluate asymptotics of the wave functions at boundary points in the case of a boundary conditions of the third-type for the above problems.

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1. Introduction

The KANTBP (KANTorovich Boundary Problem) versions 1.0 [1] and 2.0 [2] were intended only to calculate the energy levels, reaction matrix and radial wave functions of the bound state problem and the elastic scattering problem in the coupled-channel hyperspherical adiabatic approach, in which the original problems were reduced to a system of coupled-channel second order differential equations (CCSODEs) with respect to a radial variable on a semi-axis. The KANTBP version 3.0 [3] was intended for calculate of the energy levels, reflection and transmission amplitude matrices and corresponding wave functions of the bound state problem and scattering problem for the system of CCSODEs on a whole axis. Moreover, the scattering problem is solved under the condition that potential matrix elements in left and right asymptotic regions have only a "almost" diagonal form, and the left and right thresholds are the same. However a wider range of physical scattering problems are reduced to a system of CCSODEs with non-diagonal potential matrix elements in the left and/or right asymptotic regions and different left and right thresholds. The purpose of this version is to provide a computational program for calculating the reflection and transmission amplitude matrices and corresponding wave functions of the scattering spectrum problem thus covering a wider range of physical scattering problems.

The KANTBP 3.1 extends the framework of the previous versions of KANTBP for the case of the scattering problem. As in [3], it calculates the reflection and transmission amplitude matrices and corresponding wave functions of the continuous spectrum of the boundary-value problem for the system of CCSODEs on finite intervals of the variable $z \in [z_{\min}, z_{\max}]$ using a general homogeneous boundary condition of the third-type at $z = z_{\min}$ and $z = z_{\max}$. The third-type boundary conditions are formulated for the continuous problems under consideration by using known asymptotes for a set of linearly independent asymptotic regular and irregular solutions in the open channels and a set of linearly independent regular asymptotic solutions in the closed channels, respectively. We have considered more general cases, namely, in left and right asymptotic regions $z \le z_{\min}$ and $z \ge z_{\max}$ the potential matrix elements are non-diagonal and constant or weakly dependent on the variable z; the left and right thresholds are different, and the left and right threshold values may not be known in advance.

We have applied the new approach to the computation of sub-barrier and above-barrier fusion cross sections as well as the astrophysical S factor of some reactions, to study the deep sub-barrier fusion hindrance phenomenon in [5,6], and study of fast fission and quasifission in the ^{40}Ca+^{208}Pb reaction leading to the formation of the transfermium nucleus ^{248}No [7]. The results obtained using KANTBP 3.1 and the modified Numerov method in the CCFULL program [8], the Gauss reduction method in the NRV project [9–11] are compared.

Benchmark calculations for the fusion cross sections of ^{36}S+^{48}Ca, ^{64}Ni+^{100}Mo reactions, which are studied in [5], are presented. In our previous study, the fusion cross sections are calculated at the experimental incident energy in order to compare with the data for ^{36}S+^{48}Ca,

^{64}Ni+^{100}Mo reactions, while in this work they are calculated at $\Delta E = 0.1$ MeV for a strict test. The calculated fusion cross sections are also compared with those obtained by the CCFULL program [8], and the advantage of KANTBP 3.1 is more prominent. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions of the exact solvable wave-guide model considered in [12], and the fusion cross sections and mean angular momenta of the ^{16}O+^{144}Sm reaction.

The paper is organized as follows. In Section 2 we give a brief overview of the problem. A description of the KANTBP 3.1 program is given in Section 3. Benchmark calculations and test desk are given in Section 4.

2. Physical scattering asymptotic forms of solutions in longitudinal coordinates and the scattering matrix

In the Kantorovich approach [1,4], a multidimensional Schrödinger equation is reduced to a finite set of N ordinary second-order differential equations on the finite interval $z \in (z_{\min}, z_{\max})$ for the partial solution $\boldsymbol{\chi}^{(j)}(z) = \left(\chi_1^{(j)}(z), \ldots, \chi_N^{(j)}(z)\right)^T$

$$\left(-\mathbf{I}\frac{1}{z^{d-1}}\frac{d}{dz}z^{d-1}\frac{d}{dz} + \mathbf{V}(z) + \mathbf{Q}(z)\frac{d}{dz} + \frac{1}{z^{d-1}}\frac{d\,z^{d-1}\mathbf{Q}(z)}{dz} - 2E\,\mathbf{I}\right)\boldsymbol{\chi}^{(j)}(z) = 0. \tag{1}$$

Here $\mathbf{I}$, $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ are the unit, real valued symmetric and antisymmetric $N \times N$ matrices, respectively. Below we consider only the scattering problem with $d = 1$.

The matrix-solution $\boldsymbol{\Phi}_\nu(z) = \boldsymbol{\Phi}(z)$, describing the incidence wave of the particle and its scattering, which has the asymptotic form "incident wave + outgoing waves", is

$$\boldsymbol{\Phi}_\nu(z) = \begin{cases} \begin{cases} \mathbf{Y}^{(+)}(z)\mathbf{T}_\nu, & z \ge z_{\max}, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_\nu, & z \le z_{\min}, \end{cases} & \nu = \rightarrow, \\ \begin{cases} \mathbf{Y}^{(-)}(z) + \mathbf{Y}^{(+)}(z)\mathbf{R}_\nu, & z \ge z_{\max}, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_\nu, & z \le z_{\min}, \end{cases} & \nu = \leftarrow, \end{cases} \tag{2}$$

where $\nu = \rightarrow$ and $\nu = \leftarrow$ denote the initial direction of particle motion along the z axis; $\mathbf{R}_\rightarrow$ of the dimension $N_o^L \times N_o^L$ and $\mathbf{R}_\leftarrow$ of the dimension $N_o^R \times N_o^R$ are the reflection matrices, $\mathbf{T}_\rightarrow$ of the dimension $N_o^R \times N_o^L$ and $\mathbf{T}_\leftarrow$ of dimension $N_o^L \times N_o^R$ are the transmission matrices; $\boldsymbol{\Phi}_\leftarrow(z) = \{\boldsymbol{\chi}^{(j)}(z)\}_{j=1}^{N_o^R}$ and $\boldsymbol{\Phi}_\rightarrow(z) = \{\boldsymbol{\chi}^{(j)}(z)\}_{j=1}^{N_o^L}$; N_o^L and N_o^R are the number of the open channels at $z \le z_{\min}$ and $z \ge z_{\max}$.

Let $\mathbf{Q}(z) = 0$, and the $\mathbf{V}(z)$ matrix is constant or weakly dependent on the variable z in the vicinity of the asymptotic regions $z \le z_{\min}$ and $z \ge z_{\max}$. In this case, the open channel asymptotic vector solutions at $\lambda_{i_o}^{L,R} < 2E$, $i = i_o = 1, \ldots, N_o^{L,R}$, have the form:

$$\mathbf{X}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath\, p_{i_o}^L z\right)}{\sqrt{p_{i_o}^L}}\boldsymbol{\Psi}_{i_o}^L, \quad p_{i_o}^L = \sqrt{2E - \lambda_{i_o}^L}, \quad z \le z_{\min},$$
$$\mathbf{Y}_{i_o}^{(\pm)}(z) \to \frac{\exp\left(\pm\imath\, p_{i_o}^R z\right)}{\sqrt{p_{i_o}^R}}\boldsymbol{\Psi}_{i_o}^R, \quad p_{i_o}^R = \sqrt{2E - \lambda_{i_o}^R}, \quad z \ge z_{\max}. \tag{3}$$

The closed channels asymptotic vector solutions at $\lambda_{i_c}^{L,R} \ge 2E$, $i = i_c = N_o^{L,R} + 1, \ldots, N$, are as follows:

$$\mathbf{X}_{i_c}^{(-)}(z) \to \exp\left(+\sqrt{\lambda_{i_c}^L - 2E}z\right)\boldsymbol{\Psi}_{i_c}^L, \quad z \le z_{\min}, \quad \nu = \leftarrow,$$
$$\mathbf{Y}_{i_c}^{(+)}(z) \to \exp\left(-\sqrt{\lambda_{i_c}^R - 2E}z\right)\boldsymbol{\Psi}_{i_c}^R, \quad z \ge z_{\max}, \quad \nu = \rightarrow. \tag{4}$$

Here $\lambda_i^{L,R}$ and $\boldsymbol{\Psi}_i^{L,R} = \{\Psi_{1i}^{L,R}, \ldots, \Psi_{Ni}^{L,R}\}^T$ are the solutions of algebraic eigenvalue problems with the matrices $\mathbf{V}^L = V(z_{\min})$ and $\mathbf{V}^R = V(z_{\max})$ of the dimension $N \times N$ for entangled channels

$$\mathbf{V}^{L,R}\boldsymbol{\Psi}_i^{L,R} = \lambda_i^{L,R}\boldsymbol{\Psi}_i^{L,R}, \quad (\boldsymbol{\Psi}_i^{L,R})^T\boldsymbol{\Psi}_j^{L,R} = \delta_{ij}. \tag{5}$$

In addition, the eigenvalues $\lambda_i^{L,R}$ are ordered in ascending order, and the maximum element of the eigenvector $\boldsymbol{\Psi}_i^{L,R}$ in the absolute value is positive. The left N_o^L and right N_o^R numbers of open channels are defined as:

$$N_o^L = \max_{2E > \lambda_j^L} j \le N, \quad N_o^R = \max_{2E > \lambda_j^R} j \le N. \tag{6}$$

We also consider the case when the $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices have the following asymptotic behavior

$$V_{ij}(z) = \left(\epsilon_j^L + \frac{2Z_j^L}{z}\right)\delta_{ij} + O(z^{-l}), \quad l > 1, \quad Q_{ij}(z) = O(z^{-l}), \quad l \ge 1, \quad z \le z_{\min}, \tag{7}$$

and/or

$$V_{ij}(z) = \left(\epsilon_j^R + \frac{2Z_j^R}{z}\right)\delta_{ij} + O(z^{-l}), \quad l > 1. \quad Q_{ij}(z) = O(z^{-l}), \quad l \ge 1, \quad z \ge z_{\max}. \tag{8}$$

In this case, we usually have orthogonal channels. We put $V^L_{ij}=\epsilon^L_i\delta_{ij}$ and/or $V^R_{ij}=\epsilon^R_i\delta_{ij}$, and the eigenvalues λ^L_i and/or λ^R_i are ordered in ascending order of the thresholds ϵ^L_i and/or ϵ^R_i, and the corresponding eigenvectors $\mathbf{\Psi}^L_i$ and/or $\mathbf{\Psi}^R_i$ are columns of the permutated unit matrix $\mathbf{I}$. In these cases, the open and closed channel asymptotic vector solutions have the form:

$$\mathbf{X}^{(\pm)}_{i_o}(z)\to\frac{\exp\left(\pm\imath\left(p^L_{i_o}z-\frac{Z^L_j}{p_{i_o}}\ln(2p^L_{i_o}|z|)\right)\right)}{\sqrt{p^L_{i_o}}}\mathbf{\Psi}^L_{i_o},\quad p^L_{i_o}=\sqrt{2E-\lambda^L_{i_o}},\quad z\le z_{\min},$$
$$\mathbf{X}^{(-)}_{i_c}(z)\to\exp\left(+\left(p^L_{i_c}z+\frac{Z^L_j}{p_{i_c}}\ln(2p^L_{i_c}|z|)\right)\right)\mathbf{\Psi}^L_{i_c},\quad p^L_{i_c}=\sqrt{\lambda^L_{i_c}-2E}, \tag{9}$$

and/or

$$\mathbf{Y}^{(\pm)}_{i_o}(z)\to\frac{\exp\left(\pm\imath\left(p^R_{i_o}z-\frac{Z^R_j}{p_{i_o}}\ln(2p^R_{i_o}|z|)\right)\right)}{\sqrt{p^R_{i_o}}}\mathbf{\Psi}^R_{i_o},\quad p^R_{i_o}=\sqrt{2E-\lambda^R_{i_o}},\quad z\ge z_{\max},$$
$$\mathbf{Y}^{(+)}_{i_c}(z)\to\exp\left(-\left(p^R_{i_c}z+\frac{Z^R_j}{p_{i_c}}\ln(2p^R_{i_c}|z|)\right)\right)\mathbf{\Psi}^R_{i_c},\quad p^R_{i_c}=\sqrt{\lambda^R_{i_c}-2E}, \tag{10}$$

where j is the element number of the eigenvector $\mathbf{\Psi}^L_i$ and/or $\mathbf{\Psi}^R_i$, which is 1.

The reflection $\mathbf{R}_v$ and transmission $\mathbf{T}_v$ matrices, and the solution $\mathbf{\Phi}_v(z)$ are calculated by the same methods, described in [4]. The scattering matrix $\mathbf{S}$

$$\mathbf{S}=\begin{pmatrix}\mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow}\\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow}\end{pmatrix} \tag{11}$$

is composed of reflection and transmission matrices. Similar, as in [4], it is easy to show that the scattering matrix (11) is symmetric and unitary. Note that if $N^L_o=0$ (or $N^R_o=0$), then $\mathbf{S}=\mathbf{R}_{\leftarrow}$ (or $\mathbf{S}=\mathbf{R}_{\rightarrow}$).

In addition, it should be noted that the open channel asymptotic vector solutions $\mathbf{X}^{(\pm)}(z)$ and $\mathbf{Y}^{(\pm)}(z)$ satisfy the relations

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\mp)}(z),\mathbf{X}^{(\pm)}(z))=\pm2\imath\mathbf{I}^L_{oo},\quad \mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\pm)}(z),\mathbf{X}^{(\pm)}(z))=\mathbf{0}^L_{oo},$$
$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{Y}^{(\mp)}(z),\mathbf{Y}^{(\pm)}(z))=\pm2\imath\mathbf{I}^R_{oo},\quad \mathbf{Wr}(\mathbf{Q}(z);\mathbf{Y}^{(\pm)}(z),\mathbf{Y}^{(\pm)}(z))=\mathbf{0}^R_{oo}, \tag{12}$$

where $\mathbf{I}^{L,R}_{oo}$ is the unit $N^{L,R}_o\times N^{L,R}_o$ matrix, and $\mathbf{0}^{L,R}_{oo}$ is the zero $N^{L,R}_o\times N^{R,L}_o$ matrix, and $\mathbf{Wr}(\bullet;\mathbf{a}(z),\mathbf{b}(z))$ is the generalized Wronskian with a long derivative defined as

$$\mathbf{Wr}(\bullet;\mathbf{a}(z),\mathbf{b}(z))=\mathbf{a}^T(z)\left(\frac{d\mathbf{b}(z)}{dz}-\bullet\mathbf{b}(z)\right)-\left(\frac{d\mathbf{a}(z)}{dz}-\bullet\mathbf{a}(z)\right)^T\mathbf{b}(z). \tag{13}$$

This Wronskian is used to estimate the desirable accuracy of asymptotic expansions (3), (9), (10). Then the following properties of the reflection and transmission matrices are held:

$$\mathbf{T}^{\dagger}_{\rightarrow}\mathbf{T}_{\rightarrow}+\mathbf{R}^{\dagger}_{\rightarrow}\mathbf{R}_{\rightarrow}=\mathbf{I}^L_{oo},\quad \mathbf{T}^{\dagger}_{\leftarrow}\mathbf{T}_{\leftarrow}+\mathbf{R}^{\dagger}_{\leftarrow}\mathbf{R}_{\leftarrow}=\mathbf{I}^R_{oo},$$
$$\mathbf{T}^{\dagger}_{\rightarrow}\mathbf{R}_{\leftarrow}+\mathbf{R}^{\dagger}_{\rightarrow}\mathbf{T}_{\leftarrow}=\mathbf{0}^L_{oo},\quad \mathbf{R}^{\dagger}_{\leftarrow}\mathbf{T}_{\rightarrow}+\mathbf{T}^{\dagger}_{\leftarrow}\mathbf{R}_{\rightarrow}=\mathbf{0}^R_{oo},$$
$$\mathbf{T}^T_{\rightarrow}=\mathbf{T}_{\leftarrow},\quad \mathbf{R}^T_{\rightarrow}=\mathbf{R}_{\rightarrow},\quad \mathbf{R}^T_{\leftarrow}=\mathbf{R}_{\leftarrow}. \tag{14}$$

It means that the scattering matrix (11) is symmetric and unitary.

Remark 1. Depending on the physical statement of the problem, the asymptotic form of the matrix-solution may differ from (2) due to additional phase shifts, signs, etc. (for example, see Eq. (27)). Then the required reflection $\hat{\mathbf{R}}_v$ and transmission $\hat{\mathbf{T}}_v$ matrices and the corresponding matrix-solution $\hat{\mathbf{\Phi}}_v(z)$ are expressed as a linear combination of the calculated reflection $\mathbf{R}_v$ and transmission $\mathbf{T}_v$ matrices and the corresponding matrix-solution $\mathbf{\Phi}_v(z)$:

$$\hat{\mathbf{\Phi}}_v(z)=\mathbf{\Phi}_v(z)\mathbf{U}_v,\quad \hat{\mathbf{R}}_v=\pm\mathbf{U}_v\mathbf{R}_v\mathbf{U}_v,\quad \hat{\mathbf{T}}_{\leftarrow}=\mathbf{U}_{\rightarrow}\mathbf{T}_{\leftarrow}\mathbf{U}_{\leftarrow},\quad \hat{\mathbf{T}}_{\rightarrow}=\mathbf{U}_{\leftarrow}\mathbf{T}_{\rightarrow}\mathbf{U}_{\rightarrow}, \tag{15}$$

where $\mathbf{U}_{\rightarrow}$ and $\mathbf{U}_{\leftarrow}$ are the known symmetric and unitary $N^L_o\times N^L_o$ and $N^R_o\times N^R_o$ matrices.

Eq. (1) with asymptotic boundary conditions (2) is solved by the finite element method using high-order accuracy approximations as in previous versions of the KANTBP program. More detailed information on the construction of high-order approximations of the finite element method on non-uniform grids is given in [1].

3. Description of the KANTBP 3.1 program

The KANTBP program is called from the main routine (supplied by the user) which sets the dimensions of the arrays and is responsible for the input data. The KANTBP program does not require installation. A description of all subroutines can be found in comments in the program source code. Users can also find instructions on how to compile KANTBP in the README file.

The calling sequence for the KANTBP subroutine is:

```
 CALL KANTBP(TITLE,IPTYPE,ISC,ISCAT,NROOT,MDIM,IDIM,NPOL,
1            RTOL,NITEM,SHIFT,IPRINT,IPRSTP,NMESH,RMESH,
2            NDIR,NDIL,NMDIL,THRSHL,THRSHR,IBOUND,FNOUT,
3            IOUT,POTEN,IOUP,FMATR,IOUM,EVWFN,IOUF)
```

In the present program each array declarator is written in terms of the symbolic names of constants. These constants are defined in the following PARAMETER statement in the main routine:

PARAMETER (NMESHM=111,MDIMM=111)

Here

- NMESHM is the maximal dimension of the DOUBLE PRECISION array RMESH, and NMESHM $\geq$ NMESH.
- NMESH is the dimension of the DOUBLE PRECISION array RMESH, containing information about the subdivision of the longitudinal interval $[z_{\min}, z_{\max}]$ on subintervals and the number of elements on each of them. NMESH is always odd and ≥ 3.
- MDIMM is the maximal dimension of the DOUBLE PRECISION array THRSHL, THRSHR and INTEGER array NDIL, containing information about a set of left and right threshold values and numbers of coupled differential equations, respectively, and MDIMM $\geq$ MDIM.

When solving the reflection and transmission matrices, the case NOPENR = 0 or NOPENL = 0 may arise. Therefore, the flag ISC (from KANTBP 3.0 [3]) for performing the calculation of the reflection and transmission matrices takes into account the following cases:

- = 1 – if NOPENR $>$ 0, the calculation of the reflection matrix is carried out only with the direction $v = \leftarrow$. If NOPENL $>$ 0, the calculation of the transmission matrix is carried out additionally. The properties of the reflection and transmission matrices are also verified. If NOPENR = 0, the message NO RIGHT OPEN CHANNELS is printed.
  = 2 – if NOPENL $>$ 0, the calculation of the reflection matrix is carried out only with the direction $v = \rightarrow$. If NOPENR $>$ 0, the calculation of the transmission matrix is carried out additionally. The properties of the reflection and transmission matrices are also verified. If NOPENL = 0, the message NO LEFT OPEN CHANNELS is printed.
  = 3 – if NOPENR $>$ 0 and NOPENL $>$ 0, the calculation of the reflection and transmission matrices is carried out with both directions $v = \leftarrow$ and $v = \rightarrow$. The properties of the reflection and transmission matrices are also verified.

We have added a new flag ISCAT for performing the calculation of the left THRSHL and right THRSHR threshold values:

- = 1 – $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices have asymptotic behavior (7) and (8) at $z \leq z_{\min}$ and $z \geq z_{\max}$, respectively. In this case, the user must set both the left THRSHL and right THRSHR threshold values.
  = 2 – $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices have asymptotic behavior (7) at $z \leq z_{\min}$, and $\mathbf{Q}(z) = 0$ and $\mathbf{V}(z)$ is the constant matrix at $z \geq z_{\max}$. In this case, the user must set the left THRSHL threshold values, and the right THRSHR values are calculated by the program.
  = 3 – $\mathbf{Q}(z) = 0$ and $\mathbf{V}(z)$ is the constant matrix at $z \leq z_{\min}$, the $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices have the asymptotic behavior (8) at $z \geq z_{\max}$. In this case, the user must set the right THRSHR threshold values, and left THRSHL threshold values are calculated by the program.
  = 4 – $\mathbf{Q}(z) = 0$ and $\mathbf{V}(z)$ is the constant matrix at $z \leq z_{\min}$ and $z \geq z_{\max}$. In this case, the user does not set the left THRSHL and right THRSHR threshold values, they are calculated by the program.

The meaning of all arguments, except for those above, is presented in [1,4].

Output data

The results of the calculation of the reflection and transmission matrices and corresponding wave functions are written using unformatted segmented records into file EVWFN, according to the following operator:

```
 WRITE(IOUF) NDIM,NN,NL,NR,NGRID,((RR(I,J),I=1,NR),J=1,NR),
1                                ((TT(I,J),I=1,NL),J=1,NR),
1            (XGRID(I),I=1,NGRID),((R(I,J),I=1,NN),J=1,NR)
```

In the above, the parameters presented in the WRITE statement have the following meaning:

- NDIM is the number of coupled equations,
- NGRID is the number of finite-element grid points,
- NN = NGRID $\times$ NDIM,
- NL and NR are the numbers of open channels: NL = NOPENL, NR = NOPENR for $v = \leftarrow$, NL = NOPENR, NR = NOPENL for $v = \rightarrow$,
- Arrays RR and TT contain the calculated values of reflection and transmission matrices,
- Array XGRID contains the values of the finite-element grid points,
- Array R contains NR eigenfunctions each per NN elements in length stored (see the scheme in [1]).

User-supplied subroutines

```
      SUBROUTINE ASYMSL(ZMIN,ZMAX,NDIM,NOPENL,NOPENR,SHIFT,THRSHL,
     1                  THRSHR,EIGL,EIGR,PREGL,DREGL,PREGR,PIRRR,DREGR,
     2                  DIRRR,IOUT)
```

- ASYMSL is the name of the subroutine for the scattering problem, $\mathbf{\Phi}_{\leftarrow}(z)$, which calculates the regular $\mathbf{Y}^{(-)}(z) \equiv$ PREGR, irregular $\mathbf{Y}^{(+)}(z) \equiv$ PIRRR asymptotic rectangle-solutions and their derivatives DREGR, DIRRR, respectively, at $z = z_{\max}$, and the regular $\mathbf{X}^{(-)}(z) \equiv$ PREGL asymptotic square-solution and its derivative DREGL at $z = z_{\min}$.

```
      SUBROUTINE ASYMSR(ZMIN,ZMAX,NDIM,NOPENL,NOPENR,SHIFT,THRSHL,
     1                  THRSHR,EIGL,EIGR,PREGR,DREGR,PREGL,PIRRL,DREGL,
     2                  DIRRL,IOUT)
```

- ASYMSR is the name of the subroutine for the scattering problem, $\mathbf{\Phi}_{\rightarrow}(z)$, which calculates the regular $\mathbf{X}^{(+)}(z) \equiv$ PREGL, irregular $\mathbf{X}^{(-)}(z) \equiv$ PIRRL asymptotic rectangle-solutions and their derivatives DREGL, DIRRL, respectively, at $z = z_{\min}$, and the regular $\mathbf{Y}^{(+)}(z) \equiv$ PREGR asymptotic square-solution and its derivative DREGR at $z = z_{\max}$.

In the above user-supplied subroutines, the arrays EIGL and EIGR contain the eigenvectors $\mathbf{\Psi}_i^L$ and $\mathbf{\Psi}_i^R$, SHIFT contains the given double energy spectrum value. *To set third-type boundary conditions at both points $z_{\min}$ and $z_{\max}$, flags IBOUND and IDIM always should be 8 and 1, respectively.* All the parameters, except the regular and irregular asymptotic solutions and their derivatives, should not be changed by subroutines ASYMSL and ASYMSR.

4. Benchmark calculations and test desk

4.1. Exact solvable wave-guide model

For example we consider the multichannel scattering problem for the Schrödinger equation of the exact solvable wave-guide problem [12]

$$\left(-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + U(y,z) - 2E\right)\Psi(y,z) = 0 \tag{16}$$

in the 2D domain $\Omega_{yz} = \{y \in (0,\pi), z \in (-\infty,+\infty)\}$, with the potential

$$U(y,z) = \{0,\ z < -2;\ -2y,\ |z| \le 2;\ 2y,\ z > 2\}\,. \tag{17}$$

We seek for the solution in the form of the expansion

$$\Psi(y,z) = \sum_{i=1}^{N} B_i(y)\Phi_i(z) \tag{18}$$

in the set of basis functions $B_i(y) = \sqrt{2/\pi}\sin(iy)$, leading to the system of Eq. (1) with $Q_{ij}(z) = 0$ and the effective potentials $V_{ij}(z)$:

$$V_{ij}(z) = \int_0^{\pi} dy B_i(y)U(y,z)B_j(y) = i^2\delta_{ij} + \left\{0,\ z<-2;\ -2,\ |z|\le 2;\ 2,\ z>2\right\} \times \left\{\pi/2,\ i=j;\ 0,\ \text{even}\ i-j;\ \frac{-8ij}{\pi(i^2-j^2)^2},\ \text{odd}\ i-j\right\}. \tag{19}$$

It can be seen from (19) that only the diagonal elements are nonzero in the matrix elements $V_{ij}(z)$ for $z < -2$, however, they contain nonzero off-diagonal elements for $z > 2$. The considered system at $N = 6$ has a set of threshold energies that are different for the left- and right-hand asymptotic regions of the z-axis: $\lambda_i^{(L)} = \{1, 4, 9, 16, 25, 36\}$ and $\lambda_i^{(R)} = \{3.7422604996,\ 7.2420582214,\ 12.2164845016,\ 19.1886881493,\ 28.1736887739,\ 39.2863757754\}$. The solutions of boundary value problems for system of ODEs (1) with piecewise constant potential (19) can be obtained by the method of matching the fundamental solutions (MMFS) (see Ref. [13]), which is used as a test for the algorithm and the KANTBP 3.1 program.

At given $2E = 6$ for the wave incident from the left there are two open channels $N_o^L = 2$ and for the wave incident from the right there is one open channel $N_o^R = 1$. The desired **S**-matrix (11) takes the form

$$\mathbf{S} = \left(\begin{array}{cc|c} 0.3588530978+0.7661295164\imath & -0.2815519545-0.0065313508\imath & -0.2427831283-0.3821154395\imath \\ -0.2815519545-0.0065313508\imath & 0.0840387795-0.4855237553\imath & -0.8035534922+0.1794207067\imath \\ \hline -0.2427831283-0.3821154395\imath & -0.8035534922+0.1794207067\imath & -0.1705387708-0.2967670235\imath \end{array}\right), \tag{20}$$

where the square $\mathbf{R}_{\rightarrow}$, $\mathbf{R}_{\leftarrow}$ and rectangular $\mathbf{T}_{\rightarrow}$, $\mathbf{T}_{\leftarrow}$ submatrices are separated by lines.

The calculations were performed with Lagrange elements of the eighth order on the finite element grid $\Omega_z = \{-20(100)20\}$, where the number of elements is indicated in parentheses (see the input file TEST1.INP for details). Note that the results obtained by the MMFS and the numerical results obtained in both intervals $z \in (-2, 2)$ and $z \in (-20, 20)$ coincide with an accuracy of the order 10^{-12} (see the output file TEST1.LPR and Appendix A). The Wronskian (12) is also satisfied with an accuracy of the order 10^{-16}.

The following values of numerical parameters and characters have been used in the test run via the supplied input file TEST1.INP:

```
&DIMS NMESH=3,MDIM=6,NDIR=1
&END
&PARAS TITLE='  REFLECTION AND TRANSMISSION MATRICES  ',
       IPTYPE=1,ISC=3,ISCAT=2,IDIM=1,NPOL=8,
       SHIFT=6D0,IPRINT=1,IPRSTP=50,
       RMESH=-20D0,100D0,20D0,
       NDIL=6,NMDIL=0,THRSHL=1.D0,4D0,9D0,16D0,25D0,36D0,IBOUND=8,
       FNOUT='TEST1.LPR',IOUT=10,POTEN='TEST1.PTN',IOUP=11,
       FMATR='TEST1.MAT',IOUM=20,EVWFN='TEST1.WFN',IOUF=21
&END
```

4.2. Formulation of the problem with diagonalization of the incoming wave boundary conditions

We solve the coupling channel equations in the isocentrifugal approximation (neglecting the Coriolis coupling of relative and internal nuclear motion of two heavy ions) on the interval $r \in (0, \infty)$ by reducing to the finite interval $r \in (r_{\min}, r_{\max})$

$$\sum_{n'=1}^{N} \left(\left(-\frac{d^2}{dr^2} - \tilde{E} \right) \delta_{nn'} + W_{nn'}(r) \right) \psi_{n'n_o}(r) = 0. \tag{21}$$

Here $\tilde{E} = 2\mu E/\hbar^2$ is the center-of-mass energy, n_o is the number of the open entrance channel with the positive relative energy $k_{n_o}^2 = \tilde{E}_{n_o} = \tilde{E} - 2\mu\epsilon_{n_o}/\hbar^2 > 0$, $n_o = 1, \ldots, N_o \le N$, and $\epsilon_1 \le \epsilon_2 \le \ldots \le \epsilon_N$ are the threshold energies (i.e., the eigenenergies of the Hamiltonian of internal motion in the harmonic approximation [8,14]), $\{\psi_{nn_o}(r)\}_{n=1}^N$ are the components of the desirable matrix-solution, $W_{nn'}(r) = W_{n'n}(r)$ are the elements of the coupled-channels matrix of the effective potentials (CCMPs) determined by

$$W_{nn'}(r) = \frac{2\mu}{\hbar^2} \left[\left(\frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n \right) \delta_{nn'} + V_{nn'}(r) \right]. \tag{22}$$

Here $\mu = A_P A_T/(A_P + A_T)$ is the reduced mass of the target and the projectile with the masses A_T and A_P and the charges Z_T and Z_P, respectively. The quantum number l is the orbital momentum of relative motion, $W_{nn'}(r \to \infty) = 2\mu\epsilon_{n_o}/\hbar^2\delta_{nn'}$.

To formulate the incoming wave boundary condition (IWBC) in the point $r = r_{\min}$ with the correct set of threshold energies, we propose that $\mathbf{W}(r)$ is the constant matrix in a vicinity of the left boundary point $r = r_{\min}$ (see Section 2). In this case, the linearly independent matrix solution (LIMS) $\{\phi_{nm}(r)\}_{n,m=1}^N$ of Eqs. (21) can be written in the form

$$\phi_{nm}(r) = A_{nm} y_m(r). \tag{23}$$

According to formulas (3), (4), in open channels at $K_m^2 = \tilde{E} - \lambda_m > 0$, $m = 1, \ldots, M_o \le N$, and in closed channels at $K_m^2 = \tilde{E} - \lambda_m \le 0$, $m = M_o + 1, \ldots, N$ the solutions $y_m(r)$, respectively, have the form:

$$y_m(r) = \frac{\exp(-\imath K_m r)}{\sqrt{K_m}}, \quad y_m(r) = \exp(|K_m| r). \tag{24}$$

Here $\mathbf{A}$ is the $N \times N$ matrix of eigenvectors and $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_N$ are the corresponding eigenvalues of the matrix $\mathbf{W} \equiv \mathbf{W}(r_{\min})$.

In this case, the matrix of the asymptotic solutions $\{\psi_{nn_o}^{as}(r)\}_{n=1}^N$ at $n_o = 1, \ldots, N_o$, of Eqs. (22), expressed by the linear combinations of the linearly independent solutions $\phi_{nm}(r)$ determined by Eqs. (23) and (24), is

$$\psi_{nn_o}^{as}(r) = \sum_{m=1}^{M_o} \phi_{nm}(r) \hat{T}_{mn_o} \equiv \sum_{m=1}^{M_o} A_{nm} y_m(r) \hat{T}_{mn_o}, \quad r \le r_{\min}, \tag{25}$$

where $\hat{T}_{mn_o} \equiv \hat{T}_{mn_o}^{(l)}$ is the matrix of desirable partial transmission amplitudes with the correct set of threshold energies $K_m^2 > 0$, $m = 1, \ldots, M_o \le N$, in exit open channels of the IWBC.

Remark 2. The LIMS (23) differs from $\{\tilde{\phi}_{nm}(r)\}_{n,m=1}^N$ subjected to the IWBC without diagonalization of the matrix $\mathbf{W} \equiv \mathbf{W}(r_{\min})$ at $r \le r_{\min}$ accepted in CCFULL program [8] with the incorrect set of threshold energies counting on the diagonal elements $W_{nn}(r_{\min})$

$$\tilde{\phi}_{nm}(r_{\min}) = \begin{cases} \exp(-\imath q_m(r_{\min}) r)\delta_{nm}, & q_m(r_{\min}) = \sqrt{\tilde{E} - W_{mm}(r_{\min})} > 0, \quad m = 1, ..., \tilde{M}_o \\ \exp(\kappa_m(r_{\min}) r)\delta_{nm}, & \kappa_m(r_{\min}) = \sqrt{W_{mm}(r_{\min}) - \tilde{E}} \ge 0, \quad m = \tilde{M}_o + 1, ..., N. \end{cases} \tag{26}$$

Note that $\{\tilde{\phi}_{nm}(r)\}_{n,m=1}^N$ is not the LIMS of Eqs. (21) at $r \le r_{\min}$.

This is the main difference between our approach and the method proposed in the CCFULL program, and the values of $K_m = \sqrt{\tilde{E} - \lambda_m}$ and $q_m(r_{\min}) = \sqrt{\tilde{E} - W_{mm}(r_{\min})}$ differ significantly at low energy values $\tilde{E}$ taking into account that some lowest eigenvalues λ_m are smaller than the corresponding lowest diagonal elements $W_{mm}(r_{\min})$. Thus, the threshold energies $(\hbar^2/(2\mu))\lambda_m$ spread much more widely

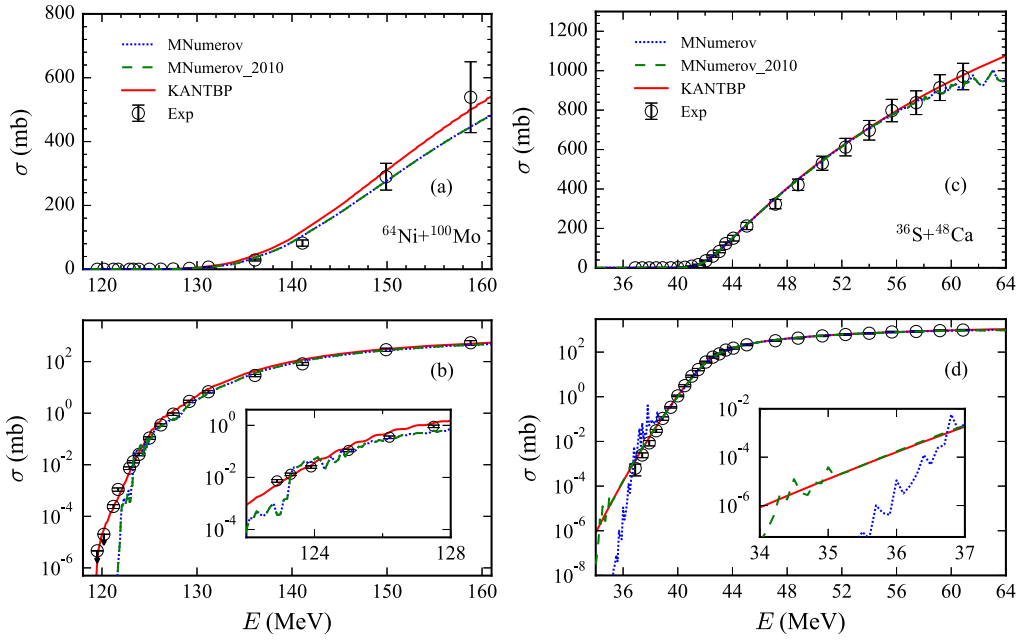

Fig. 1. (Color online) Fusion cross sections for ^{64}Ni+^{100}Mo ((a) in linear scale and (b) in logarithmic scale) and ^{36}S+^{48}Ca ((c) in linear scale and (d) in logarithmic scale). The experimental data (open circles) from Ref. [18,19] are shown for reference. The results are calculated by means of the modified Numerov (MNumerov) method in CCFULL [8] (dotted line), the improved Numerov method (MNumerov_2010) in the latest version of CCFULL [15] (dashed line) and KANTBP (solid line). All the calculations are performed at $\Delta E = 0.1$ MeV for a strict test.

than the diagonal elements $(\hbar^2/(2\mu))W_{mm}(r_{\min})$ of the coupled matrix, for example, see Fig. 3 for the fusion reaction ^{64}Ni+^{100}Mo system in Ref. [6]. It means that in our approach the number M_o of the left exit open channels from Eq. (25) will be different (conventionally increasing for a medium nuclei system with $Z_T Z_P \sqrt{\mu} > 2000$) in comparison with $\tilde{M}_o$ from Eq. (26) of the method proposed in the CCFULL program, and its true energy distribution is wider. This obstacle provides an adequate description of the experimental data of the fusion cross sections $\sigma_f(E)$ determined by Eq. (30) using correct IWBC Eq. (25) and the transmission amplitudes of Eq. (29) presented in Fig. 1 and discussed below.

At $r = r_{\max}$ the asymptotic solutions $\{\psi^{as}_{nn_o}(r)\}_{n=1}^{N}$ for $n_o = 1, \ldots, N_o$, of Eqs. (21) have the form

$$\psi^{as}_{nn_o}(r) = \frac{H^-_l(k_n r)\exp(+\imath\delta_{l,n})}{\sqrt{k_n}}\delta_{nn_o} - \frac{H^+_l(k_n r)\exp(-\imath\delta_{l,n})}{\sqrt{k_n}}\hat{R}_{nn_o}. \tag{27}$$

Here $H^{\pm}_l(k_n r) = \pm\imath F_l(\eta_n, k_n r) + G_l(\eta_n, k_n r)$ are the normalized outgoing and incoming Coulomb partial wave functions, and $F_l(\eta_n, k_n r)$ and $G_l(\eta_n, k_n r)$ are the regular and irregular Coulomb partial wave functions, $\eta_n = k_n Z_P Z_T e^2/(2E_n)$ is the Sommerfeld parameter, $E_n = E - \epsilon_n$, $\delta_{l,n} = \arg\Gamma(l+1+\imath\eta_n)$ is the Coulomb phase shift [16],

$$k_n = \sqrt{\tilde{E} - \frac{2\mu}{\hbar^2}\epsilon_n} \simeq \sqrt{\tilde{E} - \frac{2\mu}{\hbar^2}(\epsilon_n + V_{nn}(r_{\max}))}. \tag{28}$$

Here the regular and irregular Coulomb functions are calculated by the RCWFNN subroutine, which is a modified version of the RCWFN subroutine [17] for DOUBLE PRECISION accuracy, since the original RCWFN subroutine is designed for SINGLE PRECISION accuracy.

The partial tunneling probability $P_l(E)$ from the entrance open channel n_o, in particular, the ground state ($n_o = 1$) is determined by the transmission coefficient

$$P_l(E) \equiv T^{(l)}_{n_o n_o}(E) = \sum_{m=1}^{M_o} |\hat{T}_{mn_o}|^2. \tag{29}$$

Finally, the total fusion cross section is expressed as a sum over partial waves at the center of the mass energy E, which is

$$\sigma_f(E) = \sum_{l=0}^{L}\sigma^{(l)}_f(E) = \frac{\pi}{k^2_{n_o}}\sum_{l=0}^{L}(2l+1)P_l(E). \tag{30}$$

To demonstrate the working capacity of our approach and the efficiency of our KANTBP 3.1 program we analyze the couplings of relative motion only to the surface vibrations of the target nucleus, comparing our results with those obtained using CCFULL programs [8,15].

Here we present the calculations of the fusion cross sections of ^{36}S+^{48}Ca, ^{64}Ni+^{100}Mo reactions. The calculations are performed with the Woods-Saxon potential derived from the commonly adopted Akyüz-Winther parameterization, and 26 coupled channels are considered in the calculations. A description of all the necessary potentials $V^{(0)}_N(r)$, $V_{nn'}(r)$ and ϵ_n is given in our article [5], and they are calculated using subroutines of the CCFULL program [8]. In our previous study, the fusion cross sections are calculated at the experimental incident

energy to compare with the data for ^{36}S+^{48}Ca, ^{64}Ni+^{100}Mo reactions, while in this work they are calculated at $\Delta E = 0.1$ MeV for a strict test. Fig. 1 shows the fusion cross sections for ^{64}Ni+^{100}Mo ((a) in linear scale and (b) in logarithmic scale) and ^{36}S+^{48}Ca ((c) in linear scale and (d) in logarithmic scale). The experimental data (open circles) from Ref. [18,19] are also shown for reference. The results are obtained by the modified Numerov method, employed in the CCFULL program [8] (dotted line), the improved Numerov method (MNumerov_2010) in latest version of CCFULL program [15] (dashed line) and by means of KANTBP 3.1 program (solid line). The $r_{\max}$ and dr are set as 100 fm and 0.05 fm for the CCFULL calculations, and $r_{\max}$ is also set as 100 fm in the KANTBP calculation. It can be seen from Fig. 1(b,d) that there are clear fluctuations at the sub-barrier energy region of the results by the two Numerov methods, while our improved method KANTBP is stable at the whole energy region. In addition, it can be seen that the fusion cross section of ^{36}S+^{48}Ca also fluctuates in the region where the energy is greater than 58 MeV from in Fig. 1(c). Part of the reason is due to the instability of Numerov's algorithm. On the other hand, in the CCFULL program, to simplify the calculation, $r_{\min}$ is always set at the bottom of the potential pocket when $l = 0$, and the increase of $r_{\min}$ with increasing angular momentum is not considered.

As the test desk, we calculated the fusion cross sections and mean angular momenta of the ^{16}O+^{144}Sm reaction. In the first test (ccfull1.inp), the calculated fusion cross sections and mean angular momenta are comparable with the listed data published by the modified Numerov method [8]. To check the changes of the results with respect to the channels, we came up with the second test with a larger number of coupled channels (ccfull2.inp). The number of right open channels is 2 and 9 for all the input energies and l, while the number of left open channels is from 1 up 2 and from 2 up 7 depending on the input energy and l, respectively, for the first and second tests. The results of the above tests are in the output files OUTPUT1.out and OUTPUT2.out (also see Appendix B and Appendix C).

The values of the numerical parameters and characters for KANTBP 3.1 used in the above test runs are contained in the input file TEST2.INP:

```
&DIMS  NMESH=3,NDIR=1
&END
&PARAS TITLE='  REFLECTION AND TRANSMISSION MATRICES  ',
       IPTYPE=1,ISC=1,ISCAT=3,IDIM=1,NPOL=6,
       IPRINT=-1,IPRSTP=120,
       NMDIL=0,IBOUND=8,
       FNOUT='TEST2.LPR',IOUT=10,POTEN='TEST2.PTN',IOUP=11,
       FMATR='TEST2.MAT',IOUM=20,EVWFN='TEST2.WFN',IOUF=21
&END
```

The input files ccfull1.inp and ccfull2.inp:

```
16.,8.,144.,62.
1.2,-1,1.06,0
1.81,0.205,3,1
1.66,0.11,2,0
6.13,0.733,3,0
0,0.,0.3
105.1,1.1,0.75
55.,72.,1.
30,0.05
```

```
16.,8.,144.,62.
1.2,0,1.06,0
1.81,0.205,3,2
1.66,0.11,2,0
6.13,0.733,3,2
0,0.,0.3
55.1,1.1,0.75
52.,72.,1.
30,0.05
```

Remark 3. In order to carry out the above tests, the user should download the CCFULL program [8], rename adkm to ccfull.f and remove the main program and the input data from the file.

Remark 4. We used additional flags "iflagccfull", "iflagfem" in the input files nucl1.inp and nucl2.inp. If "iflagccfull", "iflagfem" are one in this line, both the modified Numerov method and the KANTBP 3.1 method are used. If one of them is zero, the corresponding calculation is switched off. The names of input file and output files, and the answers for the "Different beta_N from beta_C for this mode(n/y)?" for the CCFULL program are also included in these input files.

The input files nucl1.inp and nucl2.inp:

```
ccfull1.inp
cross1.dat
spin1.dat
OUTPUT1.dat
1,1              !iflagccfull,iflagfem
n
n
```

```
ccfull2.inp
cross2.dat
spin1.dat
OUTPUT2.dat
1,1              !iflagccfull,iflagfem
n
n
```

CRediT authorship contribution statement

O. Chuluunbaatar: Conceptualization, Software, Supervision, Visualization, Writing – original draft, Writing – review & editing. **A.A. Gusev:** Conceptualization, Software, Visualization. **S.I. Vinitsky:** Conceptualization, Software, Writing – original draft. **A.G. Abrashkevich:** Conceptualization, Software, Visualization, Writing – original draft, Writing – review & editing. **P.W. Wen:** Conceptualization, Software, Visualization, Writing – original draft. **C.J. Lin:** Conceptualization, Software, Visualization, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Test run output for wave-guide model (TEST1.LPR)

```
 PROBLEM:   REFLECTION AND TRANSMISSION MATRICES
 ********


              C O N T R O L  I N F O R M A T I O N
              -----------------------------------

     NUMBER OF DIFFERENTIAL EQUATIONS. . . . . (MDIM  ) =      6
     NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =    100
     NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =    801
     ORDER OF SHAPE FUNCTIONS. . . . . . . . . (NPOL  ) =      8
     ORDER OF GAUSS-LEGENDRE QUADRATURE. . . . (NGQ   ) =      9
     DIMENSION OF ENVELOPE SPACE . . . . . . . (IDIM  ) =      1
     BOUNDARY CONDITION CODE . . . . . . . . . (IBOUND) =      8
     DOUBLE ENERGY SPECTRUM. . . . . . . . . . (SHIFT ) =    6.00000


    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  ---------  --------  ---------  --------  --------
     1       100      -20.000   0.40000   0.05000     20.000

*******************************************************************************

     NDIM, MDIM=         6         6


              T O T A L  S Y S T E M  D A T A
              -------------------------------

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     4806
     TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =   146421
     MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =       54
     MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =       30

     NUMBER OF LEFT OPEN CHANNELS. . . . . .  (NOPENL) =      2
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      1  0.2236E+01
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      2  0.1414E+01

     NUMBER OF RIGHT OPEN CHANNELS.  . . . .  (NOPENR) =      1
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      1  0.1503E+01

*******************************************************************************

     CALCULATION OF WAVE FUNCTION WITH DIRECTION <--


         I M  P A R T  O F  W R O N S K I A N
        -------------------------------------
    -2.00000000000

         R E  P A R T  O F  RR  M A T R I X
        -----------------------------------
   -0.170538770809

         I M  P A R T  O F  RR  M A T R I X
        -----------------------------------
   -0.296767023500

         R E  P A R T  O F  TT  M A T R I X
        -----------------------------------
   -0.242783128342
   -0.803553492208
```

```
         I M  P A R T  O F  TT  M A T R I X
        ------------------------------------
   -0.382115439589
    0.179420706708

*******************************************************************************


              C H E C K  P R O P E R T I E S
          ---------------------------------------

          |RR|^2 + |TT|^2
        -------------------------
     1.00000

        M A X I M A L  A B S O L U T E  E R R O R =  0.355271E-13

          R E  P A R T:  RR^T - RR
        ----------------------------------
     0.00000

          I M  P A R T:  RR^T - RR
        ----------------------------------
     0.00000

        M A X I M A L  A B S O L U T E  E R R O R =   0.00000

        Z         R E  P A R T  O F  F U N C T I O N S
        -        -------------------------------------
    -20.0000   0.5213D-01  0.6772D+00  0.6253D-15 -0.1189D-26 -0.6446D-37 -0.1011D-46
    -17.5000   0.2306D+00 -0.5700D+00  0.4749D-13 -0.3226D-23 -0.3483D-32 -0.8945D-41
    -15.0000   0.3027D+00  0.3755D+00  0.3607D-11 -0.8750D-20 -0.1882D-27 -0.7914D-35
    -12.5000   0.2352D+00 -0.1234D+00  0.2740D-09 -0.2374D-16 -0.1017D-22 -0.7002D-29
    -10.0000   0.5911D-01 -0.1475D+00  0.2081D-07 -0.6439D-13 -0.5492D-18 -0.6195D-23
     -7.5000  -0.1442D+00  0.3959D+00  0.1581D-05 -0.1747D-09 -0.2967D-13 -0.5481D-17
     -5.0000  -0.2810D+00 -0.5836D+00  0.1201D-03 -0.4738D-06 -0.1603D-08 -0.4850D-11
     -2.5000  -0.2882D+00  0.6819D+00  0.9118D-02 -0.1285D-02 -0.8662D-04 -0.4291D-05
      0.0000  -0.4124D+00  0.1768D+00 -0.1435D-01  0.2321D-02 -0.9316D-03  0.3590D-03
      2.5000  -0.6280D+00 -0.2971D+00 -0.4394D-01 -0.6268D-02 -0.1645D-02 -0.6270D-03
      5.0000   0.4297D+00  0.1467D+00  0.2158D-01  0.4329D-02  0.9346D-03  0.4124D-03
      7.5000  -0.4715D-01 -0.1688D-01 -0.2557D-02 -0.4945D-03 -0.1080D-03 -0.4619D-04
     10.0000  -0.3510D+00 -0.1236D+00 -0.1853D-01 -0.3629D-02 -0.7896D-03 -0.3413D-03
     12.5000   0.6207D+00  0.2185D+00  0.3275D-01  0.6416D-02  0.1396D-02  0.6035D-03
     15.0000  -0.6630D+00 -0.2334D+00 -0.3499D-01 -0.6854D-02 -0.1491D-02 -0.6447D-03
     17.5000   0.4625D+00  0.1628D+00  0.2441D-01  0.4781D-02  0.1040D-02  0.4497D-03
     20.0000  -0.9258D-01 -0.3259D-01 -0.4886D-02 -0.9570D-03 -0.2082D-03 -0.9002D-04

        Z         I M  P A R T  O F  F U N C T I O N S
        -        -------------------------------------
    -20.0000  -0.2982D+00 -0.1442D+00  0.3676D-14 -0.2451D-26  0.1773D-36 -0.7770D-46
    -17.5000  -0.1961D+00  0.3930D+00  0.2792D-12 -0.6648D-23  0.9580D-32 -0.6874D-40
    -15.0000  -0.3549D-02 -0.5817D+00  0.2121D-10 -0.1803D-19  0.5176D-27 -0.6082D-34
    -12.5000   0.1907D+00  0.6813D+00  0.1611D-08 -0.4892D-16  0.2796D-22 -0.5381D-28
    -10.0000   0.2969D+00 -0.6764D+00  0.1224D-06 -0.1327D-12  0.1511D-17 -0.4761D-22
     -7.5000   0.2662D+00  0.5680D+00  0.9293D-05 -0.3600D-09  0.8163D-13 -0.4212D-16
     -5.0000   0.1126D+00 -0.3726D+00  0.7059D-03 -0.9765D-06  0.4410D-08 -0.3727D-10
     -2.5000  -0.9287D-01  0.1200D+00  0.5361D-01 -0.2649D-02  0.2383D-03 -0.3297D-04
      0.0000   0.3007D+00  0.2811D+00  0.2660D-01 -0.1192D-01 -0.5822D-03 -0.3794D-03
      2.5000   0.6810D+00  0.3115D+00  0.7312D-01  0.9182D-02  0.2041D-02  0.8150D-03
      5.0000  -0.9256D+00 -0.3211D+00 -0.4766D-01 -0.9443D-02 -0.2048D-02 -0.8942D-03
      7.5000   0.8043D+00  0.2834D+00  0.4252D-01  0.8322D-02  0.1811D-02  0.7825D-03
     10.0000  -0.3902D+00 -0.1373D+00 -0.2059D-01 -0.4033D-02 -0.8774D-03 -0.3794D-03
     12.5000  -0.1670D+00 -0.5879D-01 -0.8814D-02 -0.1727D-02 -0.3757D-03 -0.1624D-03
     15.0000   0.6630D+00  0.2334D+00  0.3499D-01  0.6854D-02  0.1491D-02  0.6447D-03
     17.5000  -0.9162D+00 -0.3225D+00 -0.4835D-01 -0.9471D-02 -0.2061D-02 -0.8909D-03
     20.0000   0.8337D+00  0.2935D+00  0.4400D-01  0.8619D-02  0.1875D-02  0.8107D-03

*******************************************************************************

     CALCULATION OF WAVE FUNCTION WITH DIRECTION -->


         I M  P A R T  O F  W R O N S K I A N
        ------------------------------------
     2.00000000000        0.00000000000
     0.00000000000        2.00000000000

         R E  P A R T  O F  RR  M A T R I X
        -----------------------------------
    0.358853097808      -0.281551954563
   -0.281551954563       0.840387795384E-01

         I M  P A R T  O F  RR  M A T R I X
        -----------------------------------
    0.766129516434      -0.653135088664E-02
   -0.653135088664E-02  -0.485523755378
```

```
        R E  P A R T  O F  TT  M A T R I X
       -----------------------------------
   -0.242783128342      -0.803553492208

        I M  P A R T  O F  TT  M A T R I X
       -----------------------------------
   -0.382115439589       0.179420706707

*******************************************************************************


             C H E C K  P R O P E R T I E S
          ---------------------------------------

           |RR|^2 + |TT|^2
          ------------------------
     1.00000      -0.599243E-13
   -0.599243E-13    1.00000

       M A X I M A L  A B S O L U T E  E R R O R =  0.212623E-12

           R E  P A R T:  RR^T - RR
          ---------------------------------
     0.00000      -0.555112E-16
    0.555112E-16    0.00000

           I M  P A R T:  RR^T - RR
          ---------------------------------
     0.00000      -0.425007E-16
    0.425007E-16    0.00000

       M A X I M A L  A B S O L U T E  E R R O R =  0.699128E-16

       Z        R E  P A R T  O F  F U N C T I O N S
       -       -------------------------------------
    -20.0000   0.3265D+00 -0.1362D+00  0.2367D+00 -0.9156D+00  0.0000D+00  0.0000D+00  0.0000D+00  0.0000D+00  0.0000D+00
               0.0000D+00  0.0000D+00  0.0000D+00
    -17.5000  -0.3818D+00 -0.2171D-01 -0.2216D+00  0.6922D+00  0.4459D-13 -0.1747D-12 -0.1256D-23  0.6860D-23 -0.1626D-32
               0.1991D-32 -0.3236D-41  0.3557D-40
    -15.0000  -0.9139D+00  0.1028D+00  0.1725D+00 -0.3628D+00  0.3387D-11 -0.1327D-10 -0.3406D-20  0.1861D-19 -0.8783D-28
               0.1076D-27 -0.2863D-35  0.3147D-34
    -12.5000  -0.1024D+01  0.1799D+00 -0.9702D-01 -0.2216D-01  0.2573D-09 -0.1008D-08 -0.9240D-17  0.5048D-16 -0.4745D-23
               0.5813D-23 -0.2533D-29  0.2785D-28
    -10.0000  -0.6623D+00  0.1740D+00  0.6668D-02  0.4037D+00  0.1954D-07 -0.7658D-07 -0.2507D-13  0.1369D-12 -0.2564D-18
               0.3141D-18 -0.2241D-23  0.2464D-22
     -7.5000   0.5353D-02  0.8781D-01  0.8470D-01 -0.7235D+00  0.1484D-05 -0.5816D-05 -0.6799D-10  0.3715D-09 -0.1385D-13
               0.1697D-13 -0.1983D-17  0.2180D-16
     -5.0000   0.6706D+00 -0.3888D-01 -0.1631D+00  0.9324D+00  0.1127D-03 -0.4418D-03 -0.1844D-06  0.1008D-05 -0.7483D-09
               0.9167D-09 -0.1755D-11  0.1929D-10
     -2.5000   0.1026D+01 -0.1476D+00  0.2165D+00 -0.9985D+00  0.8563D-02 -0.3355D-01 -0.5003D-03  0.2733D-02 -0.4043D-04
               0.4953D-04 -0.1552D-05  0.1706D-04
      0.0000   0.5474D+00  0.1260D+00  0.1091D+00 -0.3694D+00 -0.8435D-01  0.5301D-01  0.9028D-02 -0.3639D-02 -0.1432D-02
               0.2096D-02  0.3994D-04 -0.3403D-03
      2.5000   0.1293D+00  0.4856D+00 -0.4128D+00  0.4806D+00 -0.5860D-01  0.6084D-01 -0.4304D-02  0.6976D-02 -0.2145D-02
               0.2483D-02 -0.2024D-03  0.6130D-03
      5.0000   0.2233D+00 -0.3425D+00  0.5100D-01 -0.1021D+00  0.5149D-02 -0.1364D-01  0.1626D-02 -0.3086D-02  0.3103D-03
              -0.6419D-03  0.1844D-03 -0.3112D-03
      7.5000  -0.3326D+00 -0.3457D-01 -0.1188D+00 -0.1103D-01 -0.1797D-01 -0.1547D-02 -0.3481D-02 -0.3286D-03 -0.7600D-03
              -0.6978D-04 -0.3255D-03 -0.3224D-04
     10.0000   0.3300D+00  0.3924D+00  0.1161D+00  0.1382D+00  0.1739D-01  0.2072D-01  0.3409D-02  0.4058D-02  0.7415D-03
               0.8830D-03  0.3208D-03  0.3816D-03
     12.5000  -0.2059D+00 -0.6069D+00 -0.7249D-01 -0.2136D+00 -0.1087D-01 -0.3203D-01 -0.2129D-02 -0.6273D-02 -0.4632D-03
              -0.1365D-02 -0.2002D-03 -0.5901D-03
     15.0000   0.6437D-02  0.5991D+00  0.2266D-02  0.2109D+00  0.3396D-03  0.3161D-01  0.6654D-04  0.6193D-02  0.1448D-04
               0.1347D-02  0.6259D-05  0.5825D-03
     17.5000   0.1954D+00 -0.3718D+00  0.6878D-01 -0.1309D+00  0.1031D-01 -0.1962D-01  0.2020D-02 -0.3844D-02  0.4395D-03
              -0.8363D-03  0.1900D-03 -0.3615D-03
     20.0000  -0.3257D+00  0.8389D-02 -0.1146D+00  0.2953D-02 -0.1719D-01  0.4427D-03 -0.3367D-02  0.8672D-04 -0.7325D-03
               0.1887D-04 -0.3167D-03  0.8157D-05

       Z        I M  P A R T  O F  F U N C T I O N S
       -       -------------------------------------
    -20.0000   0.8986D-01 -0.1301D+00  0.7845D-02  0.4159D+00  0.0000D+00  0.0000D+00  0.0000D+00  0.0000D+00  0.0000D+00
               0.0000D+00  0.0000D+00  0.0000D+00
    -17.5000  -0.3538D+00 -0.1871D+00  0.8361D-01 -0.8999D-01  0.1302D-12  0.3266D-12 -0.2947D-23 -0.9292D-23  0.3101D-32
               0.6448D-32 -0.2740D-40 -0.7547D-40
    -15.0000  -0.6342D+00 -0.1578D+00 -0.1622D+00 -0.2497D+00  0.9890D-11  0.2481D-10 -0.7994D-20 -0.2521D-19  0.1675D-27
               0.3484D-27 -0.2424D-34 -0.6677D-34
    -12.5000  -0.6221D+00 -0.5571D-01  0.2160D+00  0.5512D+00  0.7512D-09  0.1885D-08 -0.2168D-16 -0.6837D-16  0.9052D-23
               0.1882D-22 -0.2145D-28 -0.5907D-28
    -10.0000  -0.3229D+00  0.7208D-01 -0.2367D+00 -0.7682D+00  0.5705D-07  0.1431D-06 -0.5882D-13 -0.1855D-12  0.4891D-18
               0.1017D-17 -0.1898D-22 -0.5227D-22
     -7.5000   0.1252D+00  0.1666D+00  0.2212D+00  0.8675D+00  0.4333D-05  0.1087D-04 -0.1596D-09 -0.5031D-09  0.2642D-13
               0.5494D-13 -0.1679D-16 -0.4624D-16
     -5.0000   0.5156D+00  0.1843D+00 -0.1717D+00 -0.8340D+00  0.3291D-03  0.8258D-03 -0.4329D-06 -0.1365D-05  0.1428D-08
```

```
          0.2968D-08 -0.1485D-10 -0.4091D-10
    -2.5000   0.6681D+00  0.1169D+00  0.9595D-01  0.6726D+00  0.2500D-01  0.6272D-01 -0.1174D-02 -0.3702D-02  0.7713D-04
          0.1604D-03 -0.1314D-04 -0.3620D-04
     0.0000   0.5257D+00  0.2314D+00  0.1556D+00  0.4429D+00 -0.4253D-01 -0.1694D-01  0.9521D-03 -0.6627D-02 -0.1029D-02
         -0.1783D-02 -0.1681D-03 -0.1133D-03
     2.5000   0.4298D+00  0.2942D+00 -0.1081D+00 -0.5911D-01 -0.3976D-02  0.1900D-01  0.1581D-02  0.3082D-02 -0.3855D-03
          0.4155D-04  0.2662D-03  0.2962D-03
     5.0000  -0.2691D+00 -0.5328D+00 -0.1102D+00 -0.1969D+00 -0.1790D-01 -0.3033D-01 -0.3160D-02 -0.5731D-02 -0.7125D-03
         -0.1263D-02 -0.2799D-03 -0.5290D-03
     7.5000   0.1006D+00  0.6320D+00  0.3444D-01  0.2219D+00  0.5074D-02  0.3321D-01  0.1015D-02  0.6519D-02  0.2195D-03
          0.1417D-02  0.9663D-04  0.6139D-03
    10.0000   0.1103D+00 -0.4964D+00  0.3877D-01 -0.1748D+00  0.5808D-02 -0.2620D-01  0.1139D-02 -0.5132D-02  0.2477D-03
         -0.1117D-02  0.1072D-03 -0.4827D-03
    12.5000  -0.2804D+00  0.1791D+00 -0.9872D-01  0.6305D-01 -0.1480D-01  0.9453D-02 -0.2899D-02  0.1852D-02 -0.6308D-03
          0.4029D-03 -0.2727D-03  0.1742D-03
    15.0000   0.3479D+00  0.2037D+00  0.1224D+00  0.7172D-01  0.1836D-01  0.1075D-01  0.3596D-02  0.2106D-02  0.7824D-03
          0.4583D-03  0.3383D-03  0.1981D-03
    17.5000  -0.2879D+00 -0.5120D+00 -0.1013D+00 -0.1802D+00 -0.1519D-01 -0.2702D-01 -0.2976D-02 -0.5293D-02 -0.6475D-03
         -0.1152D-02 -0.2799D-03 -0.4978D-03
    20.0000   0.1224D+00  0.6327D+00  0.4310D-01  0.2227D+00  0.6461D-02  0.3339D-01  0.1266D-02  0.6541D-02  0.2754D-03
          0.1423D-02  0.1191D-03  0.6152D-03

*******************************************************************************

             C H E C K  P R O P E R T I E S
         ---------------------------------------

         R E  P A R T:  TT_->^1 * RR_<- + RR_->^1 * TT_<-
        ---------------------------------------------------
   0.694361E-12
  -0.508538E-12

         I M  P A R T:  TT_->^1 * RR_<- + RR_->^1 * TT_<-
        ---------------------------------------------------
   0.710147E-12
   0.107225E-11

       M A X I M A L  A B S O L U T E  E R R O R =  0.118673E-11

         R E  P A R T:  TT_->^T - TT_<-
        ---------------------------------
   0.402622E-12
  -0.299427E-12

         I M  P A R T:  TT_->^T - TT_<-
        ---------------------------------
  -0.781597E-12
  -0.476535E-12

       M A X I M A L  A B S O L U T E  E R R O R =  0.879203E-12

*******************************************************************************
```

Appendix B. Test run output for the fusion cross sections (OUTPUT1.out)

```
          16 O   +           144 Sm     Fusion reaction
-------------------------------------------------
Phonon Excitation in the targ.: beta_N= 0.205, beta_C= 0.205, r0= 1.06(fm)   omega= 1.81(MeV), Lambda= 3, Nph= 1
-------------------------------------------------
Potential parameters: V0=  105.10(MeV), r0= 1.10(fm), a= 0.75(fm)
   Uncoupled barrier: Rb=10.82(fm), Vb=   61.25(MeV), Curv= 4.25(MeV)
-------------------------------------------------

                             CCFULL                      CCFULL_FEM

       Ecm (MeV)     sigma (mb)          <l>       sigma (mb)          <l>
       ---------------------------------------------------------------------
       55.00000    0.97449E-02        5.87031    0.96201E-02        5.93465
       56.00000        0.05489        5.94333        0.05335        5.99076
       57.00000        0.28583        6.05134        0.27801        6.05530
       58.00000        1.36500        6.19272        1.35113        6.14643
       59.00000        5.84375        6.40451        5.91437        6.33755
       60.00000       20.59856        6.86092       20.99607        6.82686
       61.00000       52.14435        7.81887       52.68372        7.83235
       62.00000       94.62477        9.18913       94.99815        9.21708
       63.00000      139.58988       10.65032      139.92905       10.67174
       64.00000      185.55960       11.98384      185.94640       11.99824
       65.00000      234.04527       13.13045      234.35034       13.14361
       66.00000      283.93527       14.18620      284.12497       14.19634
       67.00000      333.26115       15.21129      333.38493       15.21613
       68.00000      381.21017       16.20563      381.28717       16.20578
       69.00000      427.61804       17.16333      427.65117       17.16036
       70.00000      472.48081       18.08211      472.48114       18.07759
       71.00000      515.83672       18.96273      515.82630       18.95799
       72.00000      557.73621       19.80734      557.74591       19.80343
```

Appendix C. Test run output the fusion cross sections (OUTPUT2.out)

```
          16 O   +           144 Sm     Fusion reaction
-------------------------------------------------
Phonon Excitation in the targ.: beta_N= 0.205, beta_C= 0.205, r0= 1.06(fm)   omega= 1.81(MeV), Lambda= 3, Nph= 2
Phonon Excitation in the proj.: beta_N= 0.733, beta_C= 0.733, r0= 1.20(fm)   omega= 6.13(MeV), Lambda= 3, Nph= 2
-------------------------------------------------
Potential parameters: V0=   55.10(MeV), r0= 1.10(fm), a= 0.75(fm)
   Uncoupled barrier: Rb=10.14(fm), Vb=   64.64(MeV), Curv= 4.14(MeV)
-------------------------------------------------
```

	CCFULL		CCFULL_FEM	
Ecm (MeV)	sigma (mb)	<l>	sigma (mb)	<l>
52.00000	0.00000E+00	0.00000	0.37601E-04	3.22876
53.00000	0.00000E+00	0.00000	0.37789E-03	4.56878
54.00000	0.48512E-03	2.74497	0.27270E-02	5.12163
55.00000	0.01138	3.69681	0.01611	5.49592
56.00000	0.08730	5.90631	0.07383	6.07269
57.00000	0.24317	7.63593	0.44033	5.80180
58.00000	2.49769	7.49669	1.94929	6.46527
59.00000	5.39620	9.02205	6.81172	7.02893
60.00000	12.56862	6.33472	19.16858	7.41121
61.00000	35.56996	6.99202	44.57027	8.42200
62.00000	74.54402	9.25713	77.11841	9.39948
63.00000	99.58784	9.18304	120.37411	10.71804
64.00000	131.11721	11.02638	165.34418	11.70632
65.00000	151.97698	11.81984	212.04877	12.73508
66.00000	187.35451	12.79716	258.33768	13.79770
67.00000	222.43560	13.57383	300.23393	14.74343
68.00000	251.51478	14.17774	334.11927	15.40424
69.00000	278.95512	14.79787	371.29310	16.21770
70.00000	301.80008	15.35957	407.10211	16.99513
71.00000	322.08014	15.82657	441.70166	17.72384
72.00000	330.91749	15.96110	478.64989	18.49331

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